2-Hydroxy-3-methylbenzoic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.26

Global applicability domain: Inside

Local applicability domain index: 7.10e-01

Confidence level: 6.98e-01

Nearest Neighbors from the Training Set

Image not found
2-Hydroxy-3-methylbenzoic acid
Measured: 2.86
Predicted: 2.26

Image not found
5-Methylsalicylic acid
Measured: 2.78
Predicted: 2.27

Image not found
m-Cresotic acid
Measured: 2.99
Predicted: 2.28

Image not found
1,4-Benzenediol, 2,6-dimethyl-
Measured: 1.00
Predicted: 1.24

Image not found
2,3-dimethylhydroquinone
Measured: 1.36
Predicted: 1.36